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On Inverse Degree and Topological Indices of Graphs

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Abstract. Let G = (V, E) be a simple graph of order *n* and size *m* with maximum degree Δ and minimum degree δ . The inverse degree of a graph *G* with no isolated vertices is defined as

$$D(G) = \sum_{i=1}^n \frac{1}{d_i},$$

where d_i is the degree of the vertex $v_i \in V(G)$. In this paper, we obtain several lower and upper bounds on ID(G) of graph G and characterize graphs for which these bounds are best possible. Moreover, we compare inverse degree ID(G) with topological indices (GA_1 -index, ABC-index, Kf-index) of graphs.

1. Introduction

Throughout this paper we consider simple graphs. Let G = (V, E) be a graph with $V(G) = \{v_1, v_2, ..., v_n\}$ and |E(G)| = m. We denote by $d_i = d_G(v_i)$ the degree of vertex v_i for i = 1, 2, ..., n such that $d_1 \ge d_2 \ge \cdots \ge d_n$. The maximum vertex degree is denoted by $\Delta = \Delta(G)$ and the minimum by $\delta = \delta(G)$ in G. Other undefined notations and terminology on the graph theory can be found in [1].

Molecular descriptors play a significant role in mathematical chemistry especially in the QSPR/QSAR investigations (see [15] for some details on this topic). Among them, special place is reserved for so-called topological indices [16]. Nowadays, there exists a legion of topological indices that found particular applications in chemistry [26]. They can be classified by the structural properties of graphs used for their calculation. Here we can list some well-known topological indices of graphs as follows: Wiener index [28] (based on the distance of vertices in a graph), Hosoya index [23] (on the matching in a graph), energy [22] and Estrada index [17] (on the spectrum of a graph). Recently, a new class of topological descriptors, based

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on some properties of vertices of graph are presented. These indices are named as "geometric–arithmetic indices". The first member of this class was considered by Vukičević and Furtula [27]:

$$GA_1 = GA_1(G) = \sum_{v_i v_j \in E(G)} \frac{\sqrt{d_i d_j}}{\frac{1}{2}(d_i + d_j)}$$
(1)

In [27] it was demonstrated, on the example of octane isomers, that the GA_1 -index is well correlated with a variety of physico-chemical properties. In [4, 6, 9, 11, 27], mathematical properties of GA_1 index were studied.

Atom-bond connectivity (ABC) index is defined as follows [21]:

$$ABC(G) = \sum_{v_i v_j \in E(G)} \sqrt{\frac{1}{d_i} + \frac{1}{d_j} - \frac{2}{d_i d_j}}.$$
 (2)

The ABC index has been proven to be a valuable predictive index in the study of the heat of formation in alkanes [18]. The mathematical properties of *ABC* index were reported in [3, 7, 10, 21].

The Kirchhoff index Kf(G) of connected graph G can be written as

$$Kf = Kf(G) = n \sum_{k=1}^{n-1} \frac{1}{\mu_k},$$
(3)

where $\mu_1 \ge \mu_2 \ge \cdots \ge \mu_n = 0$ are the eigenvalues of the Laplacian matrix L(G) = D(G) - A(G), where D(G) is the diagonal matrix of vertex degrees and A(G) is the (0, 1)-adjacency matrix of graph *G*. The Kirchhoff index found noteworthy applications in chemistry as a molecular structure descriptor [19], and many of its mathematical properties have been established [5, 8].

The inverse degree of a graph G with no isolated vertices is defined [20] as

$$ID(G) = \sum_{i=1}^n \frac{1}{d_i},$$

where d_i is the degree of the vertex $v_i \in V(G)$. The inverse degree first attracted attention through conjectures of the computer program Graffiti [20]. It has been studied by several authors, see for example [13, 14, 29].

The paper is organized as follows. In Section 2, we present several lower and upper bounds on inverse degree ID(G) of graph G and characterize graphs for which these bounds are best possible. In Section 3, we compare between inverse degree ID(G) and topological indices (GA_1 -index, ABC-index, Kf-index) of graphs.

2. Lower and Upper Bounds on Inverse Degree

In this section we give some lower and upper bounds on inverse degree ID(G) of graph *G* in terms of *n*, *m*, maximum degree Δ and minimum degree δ . For this we need the following two lemmas:

Lemma 2.1. [24] Let (a_1, a_2, \ldots, a_p) be positive *p*-tuples such that there exist positive numbers A, a satisfying:

$$0 < a \le a_i \le A \, .$$

Then

$$\frac{p\sum\limits_{i=1}^{p}a_i^2}{\left(\sum\limits_{i=1}^{p}a_i\right)^2} \le \frac{1}{4}\left(\sqrt{\frac{A}{a}} + \sqrt{\frac{a}{A}}\right)^2.$$
(4)

The equality holds if and only if a = A *or*

$$q = \frac{A/a}{A/a + 1}p$$

is an integer and q of the numbers a_i coincide with a and the remaining p - q of the a_i 's coincide with $A (\neq a)$.

The following result is obtained in [2].

Lemma 2.2. [2] Let G be a graph on n vertices with m edges, maximum degree Δ and minimum degree δ . Then

$$\sum_{i=1}^n d_i^2 \leq 2m(\Delta+\delta) - n\Delta\delta$$

with equality holding if and only if G is isomorphic to a graph of two type of degrees Δ and δ .

Let Γ_1 be the class of graphs $H_1 = (V, E)$ such that there exists a positive integer p with $d_2 = d_3 = \cdots = d_p = \Delta$ and $d_{p+1} = d_{p+2} = \cdots = d_{n-1} = \delta$ where $d_i = d_{H_1}(v_i)$ with $i = 2, 3, \ldots, n-2$ as defined before. Now we are ready to give a lower bound on inverse degree ID(G) of graph G.

Theorem 2.3. Let G be a graph of order n > 2 having m edges and no isolated vertices. Then

$$ID(G) \ge \frac{\Delta + \delta}{\Delta \delta} + \sqrt{\frac{4(n-2)^3 \Delta \delta}{(\Delta + \delta)^2 \left[2m(\Delta + \delta) - n\Delta\delta - \Delta^2 - \delta^2\right]}},$$
(5)

Moreover, the equality holds if and only if G is isomorphic to a regular graph.

Proof. Setting
$$p = n - 2$$
, $A = \frac{1}{\delta}$, $a = \frac{1}{\Delta}$ and $a_i = \frac{1}{d_i}$, $i = 2, 3, ..., n - 1$; by (4) we have

$$\frac{(n-2)\sum_{i=2}^{n-1}\frac{1}{d_i^2}}{\left(\sum_{i=2}^{n-1}\frac{1}{d_i}\right)^2} \le \frac{1}{4}\left(\sqrt{\frac{\Delta}{\delta}} + \sqrt{\frac{\delta}{\Delta}}\right)^2, \quad \text{i. e., } \sum_{i=2}^{n-1}\frac{1}{d_i} \ge \sqrt{\frac{4(n-2)\Delta\delta}{(\Delta+\delta)^2}} \sum_{i=2}^{n-1}\frac{1}{d_i^2}.$$
(6)

By Arithmetic-Harmonic Mean Inequality, we have

$$\frac{\sum_{i=2}^{n-1} \frac{1}{d_i^2}}{(n-2)} \ge \frac{(n-2)}{\sum_{i=2}^{n-1} d_i^2},$$

i. e., $\sum_{i=2}^{n-1} \frac{1}{d_i^2} \ge \frac{(n-2)^2}{2m(\Delta+\delta) - n\Delta\delta - \Delta^2 - \delta^2}$ by Lemma 2.2. (7)

Using (7) in (6), we get

$$ID(G) = \sum_{i=1}^{n} \frac{1}{d_i}$$

= $\frac{1}{\Delta} + \frac{1}{\delta} + \sum_{i=2}^{n-1} \frac{1}{d_i}$
$$\geq \frac{\Delta + \delta}{\Delta \delta} + \sqrt{\frac{4(n-2)^3 \Delta \delta}{(\Delta + \delta)^2 [2m(\Delta + \delta) - n\Delta \delta - \Delta^2 - \delta^2]}}.$$
(8)

Now suppose that equality holds in (5). Then all inequalities in the above argument must be equalities. In particular, from equality in (6), we get

either
$$\Delta = \delta$$
 or $G \in \Gamma_1$.

From equality in (7), we get

$$d_2 = d_3 = \cdots = d_{n-1}$$

From equality in (8), we get that *G* has two type of degrees Δ and δ , by Lemma 2.2.

From the above, we conclude that *G* is isomorphic to a regular graph.

Conversely, one can see easily that the equality holds in (5) for regular graphs. \Box

Let Γ_2 be the class of graphs $H_2 = (V, E)$ such that $d_2 = d_3 = \cdots = d_{n-1}$ where $d_i = d_{H_2}(v_i)$ with $i = 2, 3, \ldots, n-1$ as defined before. We now give another lower and upper bounds on inverse degree ID(G) of graph *G* in terms of *n*, *m*, Δ and δ .

Theorem 2.4. Let G be a graph of order n > 2 having m edges and no isolated vertices. Then

$$\frac{\Delta+\delta}{\Delta\delta} + \frac{(n-2)^2}{2m-\Delta-\delta} \le ID(G) \le \frac{\Delta+\delta}{\Delta\delta} + \frac{(n-2)[(n-3)(\Delta^2+\delta^2)+2\Delta\delta]}{2\Delta\delta(2m-\Delta-\delta)}.$$
(9)

Moreover, the left equality holds in (9) if and only if $G \in \Gamma_2$ *and the right equality holds in (9) for regular graphs.*

Proof. Now,

$$\sum_{i=2}^{n-1} d_i \sum_{i=2}^{n-1} \frac{1}{d_i} = n-2 + \sum_{2 \le i < j \le n-1} \left(\frac{d_i}{d_j} + \frac{d_j}{d_i} \right)$$
$$= n-2 + \sum_{2 \le i < j \le n-1} \sqrt{\left(\frac{d_i}{d_j} - \frac{d_j}{d_i} \right)^2 + 4}$$
(10)

$$\geq n-2+(n-2)(n-3) \left(\operatorname{as} \left(\frac{d_i}{d_j} - \frac{d_j}{d_i} \right)^2 \geq 0 \right)$$

$$= (n-2)^2.$$
(11)

From the above, we get

$$ID(G) = \sum_{i=1}^{n} \frac{1}{d_i} \ge \frac{1}{\Delta} + \frac{1}{\delta} + \frac{(n-2)^2}{\sum_{i=2}^{n-1} d_i} = \frac{\Delta + \delta}{\Delta \delta} + \frac{(n-2)^2}{2m - \Delta - \delta}$$

Since

$$\frac{d_i}{d_j} - \frac{d_j}{d_i} \le \frac{\Delta}{\delta} - \frac{\delta}{\Delta} \text{ for } 2 \le i < j \le n - 1,$$

from (10), we get

$$\sum_{i=2}^{n-1} d_i \sum_{i=2}^{n-1} \frac{1}{d_i} \le n-2 + \sum_{2 \le i < j \le n-1} \left(\frac{\Delta}{\delta} + \frac{\delta}{\Delta}\right) = n-2 + \frac{(n-2)(n-3)}{2} \times \left(\frac{\Delta}{\delta} + \frac{\delta}{\Delta}\right).$$
(12)

Using the above relation, we get

$$\sum_{i=1}^{n} \frac{1}{d_i} = \frac{\Delta + \delta}{\Delta \delta} + \sum_{i=2}^{n-1} \frac{1}{d_i}$$
$$\leq \frac{\Delta + \delta}{\Delta \delta} + \frac{(n-2)(n-3)(\Delta^2 + \delta^2) + 2(n-2)\Delta \delta}{2\Delta \delta(2m - \Delta - \delta)}.$$

Now suppose that the equalities hold in (9). Then all inequalities in the above argument must be equalities. In particular, from equality in (11), we get

$$\left(\frac{d_i}{d_j} - \frac{d_j}{d_i}\right)^2 = 0 \text{ for } 2 \le i < j \le n - 1,$$

that is,

$$d_i = d_j$$
 for $2 \le i < j \le n - 1$, that is, $d_2 = d_3 = \cdots = d_{n-1}$

Thus we have $G \in \Gamma_2$.

From equality in (12), we get

$$d_i = \Delta$$
 and $d_j = \delta$ for $2 \le i < j \le n - 1$.

Thus we have

 $\Delta = d_2 = d_3 = \cdots = d_{n-1} = \delta$, that is, *G* is isomorphic to a regular graph.

Conversely, one can see easily that the left equality holds in (9) for graphs $G \in \Gamma_2$ and the right equality holds for regular graphs. \Box

3. Comparison Between Inverse Degree and Topological Indices of Graphs

In this section we compare inverse degree ID(G) with topological indices (GA_1 -index, ABC-index, Kf-index) of graphs. We start with an example:

Example 1. For $G = K_{10,25}$, we have

$$2d_j(d_i - d_j) \ge \sqrt{d_i(2d_i + d_j - 2)}$$

for any edge $v_i v_j \in E(G)$ with $d_i \ge d_j$.

In [12], we compare GA_1 -index and *ABC*-index for chemical trees and molecular graphs. Here we compare these two indices for general graphs.

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Theorem 3.1. Let G be a graph with degree d_i of vertex v_i , i = 1, 2, ..., n. If

$$2d_j(d_i - d_j) \ge \sqrt{d_i(2d_i + d_j - 2)}$$

for any edge $v_i v_j \in E(G)$ with $d_i \ge d_j$, then $GA_1(G) > ABC(G)$.

Proof. We can easily see that $\frac{1}{1+x} > 1 - x$ when $x \ge 1$. Therefore, for $d_i \ge d_j$, we have

$$\frac{\sqrt{d_i d_j}}{d_i + d_j} = \sqrt{\frac{d_j}{d_i}} \left(1 + \frac{d_j}{d_i}\right)^{-1} \\
> \sqrt{\frac{d_j}{d_i}} \left(1 - \frac{d_j}{d_i}\right) \\
= \sqrt{\frac{d_j}{d_i}} - \sqrt{\left(\frac{d_j}{d_i}\right)^3}.$$
(13)

Since

$$1 + \frac{y-2}{x} \le 1 + \frac{y-2}{x} + \frac{(y-2)^2}{4x^2} \text{ with } x, y \ge 1,$$

we have

$$\sqrt{1 + \frac{y-2}{x}} \le 1 + \frac{1}{2} \frac{y-2}{x}$$
.

Using the above result, we get

$$\sqrt{\frac{d_i + d_j - 2}{d_i d_j}} = \frac{1}{\sqrt{d_j}} \left(1 + \frac{d_j - 2}{d_i} \right)^{1/2} \\
\leq \frac{1}{\sqrt{d_j}} \left(1 + \frac{1}{2} \cdot \frac{d_j - 2}{d_i} \right) \\
= \frac{1}{\sqrt{d_j}} + \frac{\sqrt{d_j}}{2d_i} - \frac{1}{d_i \sqrt{d_j}}.$$
(14)

From the given condition, we have

 $2d_j(d_i - d_j) \ge \sqrt{d_i}(2d_i + d_j - 2)$ for any edge $v_i v_j \in E(G)$ with $d_i \ge d_j$.

Dividing both sides to the above inequality by $2d_i \sqrt{d_i d_j}$, we get

$$\sqrt{\frac{d_j}{d_i}\left(1-\frac{d_j}{d_i}\right)} \ge \frac{1}{\sqrt{d_j}} + \frac{\sqrt{d_j}}{2d_i} - \frac{1}{d_i\sqrt{d_j}} \text{ for any edge } v_i v_j \in E(G) \text{ with } d_i \ge d_j ,$$

that is,

$$\frac{\sqrt{d_i d_j}}{d_i + d_j} > \sqrt{\frac{d_i + d_j - 2}{d_i d_j}} \text{ for any edge } v_i v_j \in E(G) \text{ with } d_i \ge d_j \text{ , by (13) and (14) .}$$

Using the above result, we have

$$GA_1(G) = \sum_{v_i v_j \in E(G)} \frac{2\sqrt{d_i d_j}}{d_i + d_j} > \sum_{v_i v_j \in E(G)} \sqrt{\frac{1}{d_i} + \frac{1}{d_j} - \frac{2}{d_i d_j}} = ABC(G).$$

This completes the proof. \Box

We now give a relation between inverse degree ID(G) and Kirchhoff index Kf(G) of graph G.

Theorem 3.2. Let G be a connected graph of order n, m edges with minimum degree δ . If

$$2m\sqrt{n} \le (n-1)^2\,\delta,$$

then

$$Kf(G) \ge \sqrt{n} \cdot ID(G)$$

Proof. Since *G* is connected, $\mu_{n-1} > 0$. Note that

$$\sum_{i=1}^{n-1} \mu_i = 2m.$$

From the definition of Kirchhoff index, we have

$$Kf(G) = \sum_{i=1}^{n-1} \frac{n}{\mu_i}$$

$$\geq n \frac{(n-1)^2}{\sum_{i=1}^{n-1} \mu_i} \text{ (by the Arithmetic-Harmonic Mean Inequality)}$$

$$= \frac{n(n-1)^2}{2m}$$

$$\geq \frac{n\sqrt{n}}{\delta} \text{ (as } 2m\sqrt{n} \le (n-1)^2\delta)$$

$$\geq \sum_{i=1}^n \frac{\sqrt{n}}{d_i} = \sqrt{n} \cdot ID(G).$$

This completes the proof. \Box

We now consider any tree *T* of order $n \ge 6$. For tree *T*, we have m = n-1 and $\delta = 1$. Then $2m\sqrt{n} \le (n-1)^2 \delta$, since $n - 1 \ge 2\sqrt{n}$ for $n \ge 6$. By Theorem 3.2, we have $Kf(T) \ge \sqrt{n} \cdot ID(T)$ for any tree *T* of order $n \ge 6$.

For $G = K_n$ ($n \ge 3$), we have

$$ID(G) = \frac{n}{n-1}$$
 and $ABC(G) = \frac{n(n-1)}{2} \cdot \frac{\sqrt{2n-4}}{(n-1)} = n\sqrt{\frac{n-2}{2}}$.

Therefore ABC(G) > ID(G). For $G = K_{1,n-1}$, we have

$$ABC(G) = \sqrt{(n-1)(n-2)} < n-1 + \frac{1}{n-1} = ID(G).$$

From the above, it is easy to see that *ABC*-index and inverse degree ID(G) are incomparable. But under certain conditions, we get the following result:

Theorem 3.3. Let *G* be a graph of order *n* with no isolated vertices. If $\delta \ge 2$, then

Proof. Now we have

$$ABC(G) = \sum_{v_i v_j \in E(G)} \sqrt{\frac{1}{d_i} + \frac{1}{d_j} - \frac{2}{d_i d_j}}$$

= $\frac{1}{2} \sum_{v_i v_j \in E(G)} \left(\sqrt{\frac{1}{d_i} + \frac{d_i - 2}{d_i d_j}} + \sqrt{\frac{1}{d_j} + \frac{d_j - 2}{d_i d_j}} \right)$
 $\geq \frac{1}{2} \sum_{v_i v_j \in E(G)} \left(\sqrt{\frac{1}{d_i}} + \sqrt{\frac{1}{d_j}} \right) \text{ (as } d_k \ge \delta \ge 2)$
 $> \frac{1}{2} \sum_{v_i v_j \in E(G)} \left(\frac{1}{d_i} + \frac{1}{d_j} \right) \text{ (as } d_k \ge \delta \ge 2)$
 $= \frac{n}{2} \ge \sum_{i=1}^n \frac{1}{d_i} = ID(G) \text{ (as } \delta \ge 2) .$

This completes the proof. \Box

From the above result, we can get immediately:

Theorem 3.4. Let \overline{G} be the complement of G with $\delta(G) \ge 2$ such that $\delta(\overline{G}) \ge 2$. Then

$$ABC(G) + ABC(\overline{G}) > ID(G) + ID(\overline{G}).$$

Proof. Since $\delta(G) \ge 2$ and $\delta(\overline{G}) \ge 2$, from Theorem 3.3, we get

 $ABC(G) + ABC(\overline{G}) > n \ge ID(G) + ID(\overline{G})$.

The following result is obtained in [4].

Lemma 3.5. [4] Let G be a connected graph of m edges with maximum vertex degree Δ and minimum vertex degree δ . Then

$$GA_1(G) \ge \frac{2m\sqrt{\Delta\,\delta}}{\Delta+\delta}$$

with equality holding if and only if G is isomorphic to a regular graph or G is isomorphic to a bipartite semiregular graph.

For $G = K_n$, we have

$$GA_1(G) = \frac{n(n-1)}{2} > \frac{n}{n-1} = ID(G).$$

Moreover, for $G = K_{1,n-1}$, we have

$$GA_1(G) = \frac{2(n-1)^{3/2}}{n} < n-1 + \frac{1}{n-1} = ID(G).$$

From the above results, we can see that inverse degree ID(G) and GA_1 -index are incomparable. But we have the following result:

Theorem 3.6. *Let G be a graph with no isolated vertices and maximum degree* Δ *, minimum degree* δ *. If the average degree*

$$\overline{d} \ge 2\sqrt{\frac{\Delta}{\delta^3}}$$
,

then

$$GA_1(G) \ge ID(G)$$
.

Proof. Let *G* be a graph with *n* vertices and *m* edges. Then we have $2m = \overline{d}n$. Now we have

$$GA_{1}(G) = \sum_{v_{i}v_{j}\in E(G)} \frac{2\sqrt{d_{i}d_{j}}}{d_{i}+d_{j}}$$

$$\geq \frac{2m\sqrt{\Delta\delta}}{\Delta+\delta} \quad (\text{ by Lemma 3.5})$$

$$\geq m\sqrt{\frac{\delta}{\Delta}}$$

$$\geq \frac{n}{\delta} \quad \left(\text{as } 2m = n\overline{d} \text{ and the condition that } \overline{d} \geq 2\sqrt{\frac{\Delta}{\delta^{3}}}\right)$$

$$\geq ID(G) \quad \text{as } d_{k} \geq \delta.$$

This completes the proof. \Box

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